

Minutes PSF MX User Meeting on ZOOM 2026-08-27

Time: 4 pm Thursday 27 August 2026

Zoom: <https://ki-se.zoom.us/j/2552303941>

Participants: Martin Moche, Herwig Schuler, Hannah Nilsson, Tulika Das, Joanna Zawacka, Tarvi Teder

§1 DECISION: Next PSF MX User Meeting

16:00 on Thursday 10 September 2026.

§2 INFORMATION: Experimentalist assignment procedures for BioMAX

To avoid BAG member friction, below is a reminder on how we assign experimentalists.

- The goal of "**§3 DECISION: Assign experimentalists**" below is to allocate experimentalists.
- Meeting participants are responsible for sharing the available beamtime, and determining who will start, share dewar shipping etc.
- Individuals absent from the meeting may receive beamtime as a courtesy from the assigned experimentalists in b) who reserve the right to refuse others from joining.

§3 DECISION: Assign experimentalists

Light source	Beamline	Date	Duration	Start	Experimentalists
MAX IV	BioMAX	2026-09-04	8 hours	16:00	HS 1, MM 2, HN 1, DD 1
Diamond	B21-SAXS	2026-09-21	24 hours	09:00	TD 3ss, 1bm, and TT 1ss Xbm

Table 1. See also <http://ki.se/en/mbb/psf-mx>. Please share sample information (UniprotID, heavy atoms, expression host) and approximate number of crystals asap after meeting.

MM will ask for a second shift of Beamtime, LiU starts and preliminary finish at 20:00.

MM ask about UV trace and longer times between SEC-SAXS injections.

§4 INFORMATION – Diamond BAG – results from AP40

Please find the result of our joint Diamond proposal submitted 17 March 2026 attached. We should prioritize sending some samples to Diamond on a regular basis – see “Peer Review Panel comments” attached. The upcoming MAX4U upgrade and unique mail-in SAXS and stable unattended MX data collection opportunities at Diamond Light Source make it worth keeping our Diamond BAG active.

§5 INFORMATION – MAX IV BAG Final Report

In mid-September, a Final MAXIV BAG report is to be submitted, and your input is required as:

- Status of potential manuscripts in preparation i.e.
 - In writing
 - Submitted
 - In Review
 - Accepted
- PDB entries on hold for publication
 - Status: In writing, Submitted, in Review, Accepted
 - Title of deposition
 - Author of deposition
- Conference contribution
 - Title of poster (Title of talk)
 - Conference name and venue
 - Participant Name
- Master or PhD thesis
 - Title of thesis
 - Author Name

Information on your publications and released PDB entries are NOT required! Since available online

§5 INFORMATION – PReSTO from Tetralith towards Arrhenius

Data transfer for pilot project NAISS 2026/3-89 from Tetralith to Arrhenius will start 14 September and be done by NSC staff. Tetralith users are recommended to review and delete data that is no longer in active use for project NAISS 2026/3-89.

Please manage your own compute and storage projects at Tetralith accordingly.

First PReSTO installations at Arrhenius at the smaller CPU partition suitable for MX and NMR is expected to be available around mid-September. Having PReSTO running on the larger GPU partitions of interest to CryoEM community will follow, however the unique [Arrhenius architecture](#) might make some familiar software's not immediately runnable at the GPU partitions. Structura has compiled CryoSPARC for architectures like Arrhenius and we hope to have our PReSTO pilot project granted at Arrhenius GPU partition for CryoEM software testing from 1st of September 2026.

Because the Arrhenius CPU partition is very small, we can expect to have less time and storage at Arrhenius CPU partition for MX and NMR as compared to Tetralith. This is not a large issue because data processing has developed in recent years and re-processing is rarely required. For MX we also have the MAX IV cluster and LUNARC Cosmos. The NMR community has only taken small steps towards PReSTO, and a few NMR software's are available at Cosmos, and slightly more NMR software at Arrhenius while replacing Tetralith.

Arrhenius PCD (Persistent Compute and Data) may benefit the NMR community familiar with NMRbox however a significant increase in NMR community engagement in PReSTO is required for this to happen.

§6 INFO: PSF in iLab - https://karolinska.corefacilities.org/service_center/show_external/3663

- ✓ Please register your research group, students, postdocs, and project numbers in iLab.
- ✓ Visit <https://staff.ki.se/research-support/research-data-management/ilab> for guidance.
- ✓ Ask cfm-support@ki.se for help.